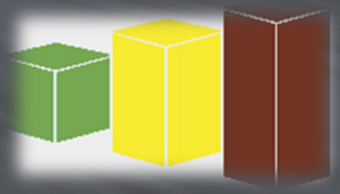
RESEARCH DATA ALLIANCE



Arbeitsprozess und Notwendigkeit einer RDA IG am Beispiel der

Interest Group Big Data Analytics

Morris Riedel et al., Forschungszentrum Juelich

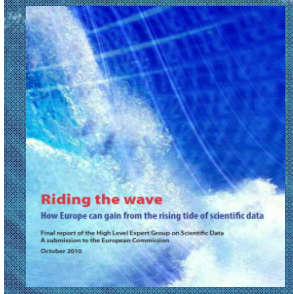
research data sharing without barriers

rd-alliance.org

20. November 2014

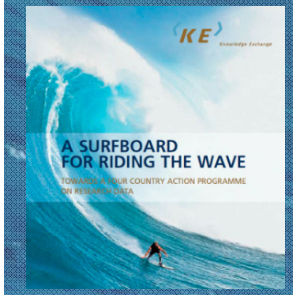
RDA – Deutschland Treffen, Deutsches GeoForschungszentrum, Potsdam

„[Scientific] Big Data Analytics“
Notwendigkeit einer konkreten RDA Interest Group



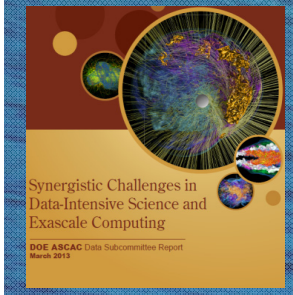
‘… problems that require high-performance data storage, **smart analytics**, transmission and mining to solve.’

[1] John Wood et al.



‘In the data-intensive scientific world, **new skills are needed for** …, **analysing**, and making available large amounts of data…’

[2] KE Partners



‘Integration of **data analytics** with exascale simulations represents a new kind of workflow…’

[3] DOE ASCAC Report

RDA
RESEARCH DATA ALLIANCE

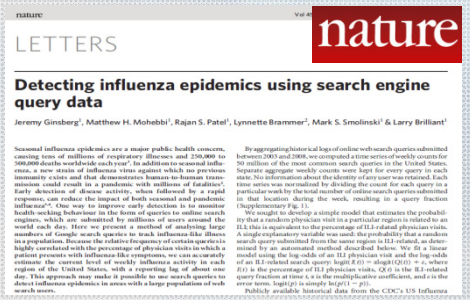
2009 – H1N1 Virus Made Headlines

Nature paper von Google Mitarbeitern

(1) Erklärt wie Google Wintergrippen schnell vorhersagen kann

(2) Nicht nur auf nationaler Ebene, auch in Regionen

(3) Möglichkeit durch „logged big data“ (Suchanfragen)


nature

LETTERS

Detecting influenza epidemics using search engine query data

Jeremy Ginsberg[1], Matthew H. Mohebbi[1], Rajan S. Patel[1], Lynnette Brammer[2], Mark S. Smolinski[2] & Larry Brilliant[1]

Seasonal influenza epidemics are a major public health concern, causing tens of millions of respiratory illnesses and 250,000 to 500,000 deaths worldwide each year[1]. In addition to seasonal influenza, a new strain of influenza virus against which no previous immunity exists and that demonstrates human-to-human transmission could result in a pandemic with millions of fatalities[2]. Early detection of disease activity, when followed by a rapid response, can reduce the impact of both seasonal and pandemic influenza[3,4]. One way to improve early detection is to monitor health-seeking behaviour in the form of queries to online search engines, which are submitted by millions of users around the world each day. Here we present a method of analysing large numbers of Google search queries to track influenza-like illness in a population. Because the relative frequency of certain queries is highly correlated with the percentage of physician visits in which a patient presents with influenza-like symptoms, we can accurately estimate the current level of weekly influenza activity in each region of the United States, with a reporting lag of about one day. This approach may make it possible to use search queries to detect influenza epidemics in areas with a large population of web search users.

By aggregating historical logs of online web search queries submitted between 2003 and 2008, we computed a time series of weekly counts for 50 million of the most common search queries in the United States. Separate aggregate weekly counts were kept for every query in each state. No information about the identity of any user was retained. Each time series was normalized by dividing the count for each query in a particular week by the total number of online search queries submitted in that location during the week, resulting in a query fraction (Supplementary Fig. 1).

We sought to develop a simple model that estimates the probability that a random physician visit in a particular region is related to an ILI. this is equivalent to the percentage of ILI-related physician visits. A single-explanatory variable was used: the probability that a random search query submitted from the same region is ILI-related, as determined by an automated method described below. We fit a linear model using the log-odds of an ILI physician visit and the log-odds of an ILI-related search query: $\text{logit}\, I(t) = \alpha \text{logit}(Q(t)) + \varepsilon$, where $I(t)$ is the percentage of ILI physician visits, $Q(t)$ is the ILI-related query fraction at time t, α is the multiplicative coefficient, and ε is the error term. $\text{logit}(p)$ is simply $\ln[p/(1-p)]$.

Publicly available historical data from the CDC's US Influenza

[7] Jeremy Ginsburg et al., ‘Detecting influenza epidemics using search engine query data’, Nature 457, 2009

“Big Data Ansätze können täuschen“

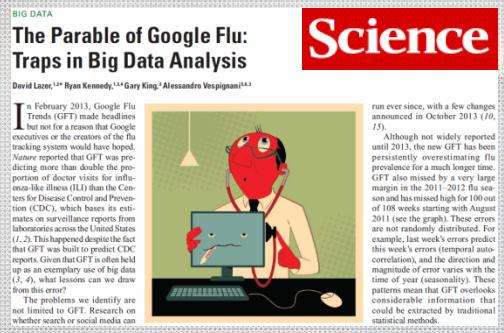
2014 – The Parable of Google Flu

Große Fehler in Vorhersage von Wintergrippen & Lessons learned

(1) Daten im wandel: Transparenz & Reproduzierbarkeit unmöglich

(2) Analyse von Ansätzen & Algorithmen den sie ändern sich

(3) Verfahren in der Community – nicht Größe nur entscheidend


BIG DATA

The Parable of Google Flu: Traps in Big Data Analysis

Science

David Lazer,[1,2]* Ryan Kennedy,[1,3,4] Gary King,[3] Alessandro Vespignani[3,4,5]

In February 2013, Google Flu Trends (GFT) made headlines but not for a reason that Google executives or the creators of the flu tracking system would have hoped. *Nature* reported that GFT was predicting more than double the proportion of doctor visits for influenza-like illness (ILI) than the Centers for Disease Control and Prevention (CDC), which bases its estimates on surveillance reports from laboratories across the United States (*1*, *2*). This happened despite the fact that GFT was built to predict CDC reports. Given that GFT is often held up as an exemplary use of big data (*3*, *4*), what lessons can we draw from this error?

The problems we identify are not limited to GFT. Research on whether search or social media can

run ever since, with a few changes announced in October 2013 (*10*, *15*).

Although not widely reported until 2013, the new GFT has been persistently overestimating flu prevalence for a much longer time. GFT also missed by a very large margin in the 2011–2012 flu season and has missed high for 100 out of 108 weeks starting with August 2011 (see the graph). These errors are not randomly distributed. For example, last week's errors predict this week's errors (temporal autocorrelation), and the direction and magnitude of error varies with the time of year (seasonality). These patterns mean that GFT overlooks considerable information that could be extracted by traditional statistical methods.

[8] David Lazer, Ryan Kennedy, Gary King, and Alessandro Vespignani, ‘The Parable of Google Flu: Traps in Big Data Analysis’, Science Vol (343), 2014

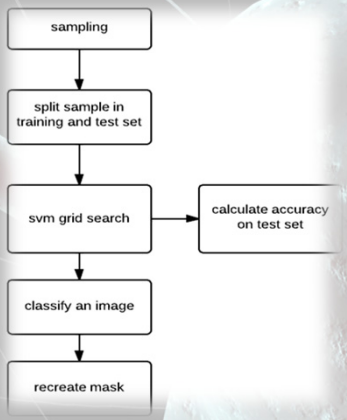
Big Data Analytics

RDA

RESEARCH DATA ALLIANCE

Analytics Prozess…
… ist komplex

Klassifikation Beispiel

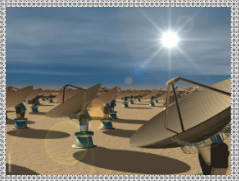


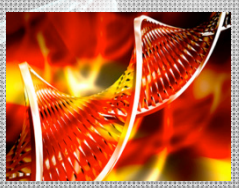
Einige Herausforderungen

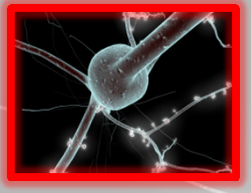
‘Sampling bias‘:
mehr Schwarz als Weiss
Pixel in „groundtruth“
„Hintergrundproblem“:
Gehirnschnitte im Eis

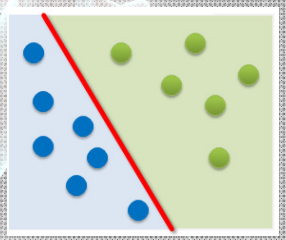
Kombination vieler Bereiche

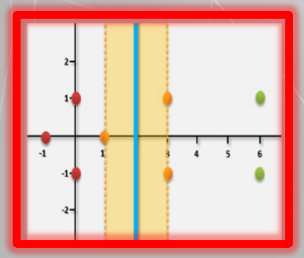
Community-basierte Methoden (⇒ right)
Skills & Toolset zur Datenanalyse (⇒ below)
Skalierbares Toolset & Infrastruktur (⇒ left)

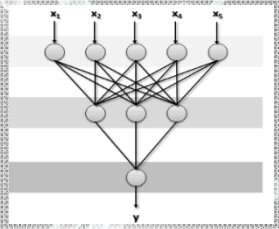










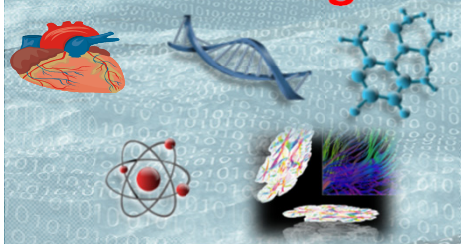


Der Komplex „Big Data“…

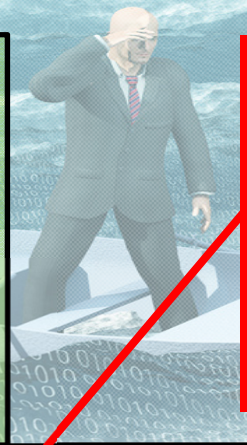
… erfordert Konzentration auf wesentliche Bereiche zum Fortschritt der Wissenschaft

Hadoop 1.0 Hadoop 2.0 Spark Dateisysteme Google DataFlow >#200 NoSQL Databases

„Bottom-Up“ Wissenschaftliche Anwendungen



Scientific Computing



“Statistical Data Mining”

Maschinelles Lernen von Daten

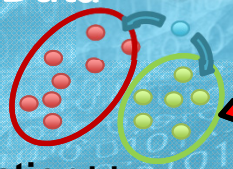
Prinzipien wie Parallelisierung

Neue HPC/HTC Algorithmen

Skalierbare Werkzeuge (“Big“)

Offene & verfügbare Ansätze

“Big Data”



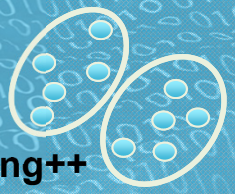
Classification++

Gruppenfokus

RESEARCH DATA ALLIANCE

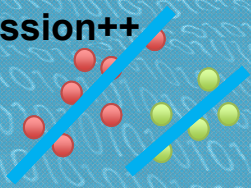
Big Data Analytics

„Open“



Clustering++

Regression++

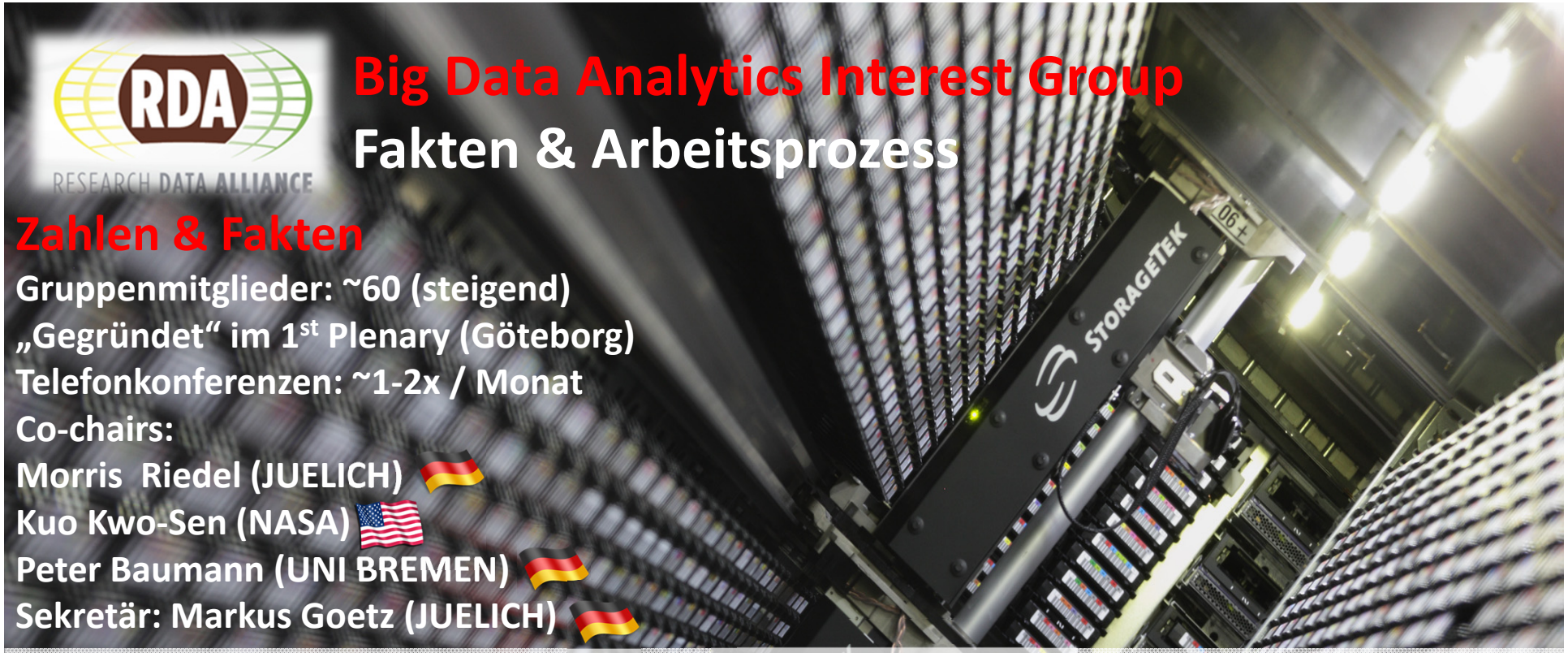


Big Data Analytics Interest Group

Fakten & Arbeitsprozess

Zahlen & Fakten

Gruppenmitglieder: ~60 (steigend)
„Gegründet“ im 1st Plenary (Göteborg)
Telefonkonferenzen: ~1-2x / Monat
Co-chairs:
Morris Riedel (JUELICH)
Kuo Kwo-Sen (NASA)
Peter Baumann (UNI BREMEN)
Sekretär: Markus Goetz (JUELICH)



Konkrete Datensätze

Algorithmen & Methoden

Technologien & Ressourcen

Wissen-schaftliche Anwendung

Big Data Analytics Gruppenprozess

„Peer-Review“

„Best Practices“

Community-basierte Empfehlungen

„Reference Data Analytics“ zur Wiederverwendung

Report (CRISP-DM)	Openly Shared Datasets	Running Analytics Code

Big Data Analytics Interest Group

RESEARCH DATA ALLIANCE

Konkretes Beispiel

Brain Data Analytics

Smart Data Innovation Lab

IT Gipfel Pressemappe

„Big Data“

Satellitenaufnahmen

JÜLICH FORSCHUNGSZENTRUM

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

[6] G. Cavallaro & M. Riedel et al., ‘Smart Data Analytics Methods for Remote Sensing Applications’, IEEE IGARSS, Quebec, Canada

„Peer-Review“

„Reference Data Analytics“ zur Wiederverwendung

Report (CRISP-DM)	Openly Shared Datasets	Running Analytics Code

Parallel Support Vector Machines (SVM)

HPC/MPI, Map-Reduce & GPGPUs

Classification Study of Land Cover Types

„Best Practices“

Community-basierte Empfehlungen

B2SHARE Store and Share Research Data

[5] EUDAT B2SHARE

πSVM

[4] piSVM

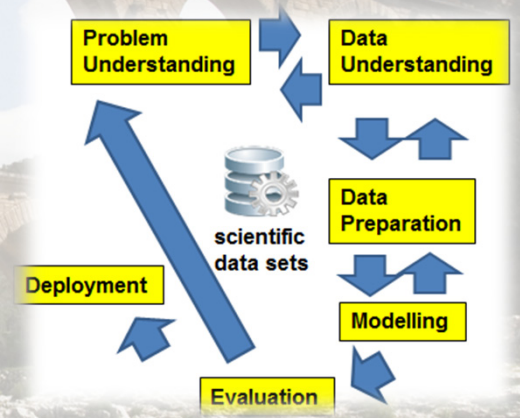
Arbeitsprozess "Systematic Big Data Analytics"

Geleitet durch Cross Industry Standard Process for Data Mining (CRISP-DM) Phasen

"Erstellung eines UCI Repository …
…für [Scientific] Big Data Analytics"

RESEARCH DATA ALLIANCE

Big Data Analytics IG &
Spin-off Big Data Infrastructure WG



[9] P. Chapman et al., CRISP-DM Guide

„Reference Data Analytics"
for reusability & learning

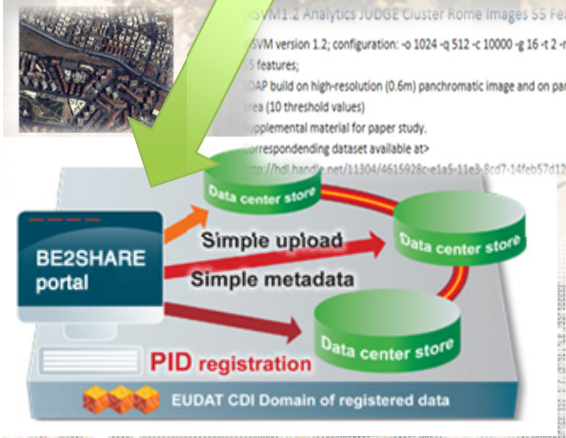
CRISP-DM Report	Openly Shared Datasets	Running Analytics Code

RESEARCH DATA ALLIANCE

Big Data Analytics IG &
Spin-off Big Data Infrastructure WG

„Reference Data Analytics“
for reusability & learning

CRISP-DM Report	Openly Shared Datasets	Running Analytics Code



[5] EUDAT B2SHARE

Link zu anderen Gruppen:

bspw. RDA Reproducability IG

Analytics Input – Vortrag in Session im Plenary 4
Gemeinsame Session in Plenary 5 vorgeschlagen

Arbeitsprozess in Richtung
“Reproduzierbare Big Data Analytics“

Link zu anderen Projekten:

Plenary 4 APARSEN Workshop

Vortrag: Data Sharing Experiences of Smart
Data Analytics Tasks in Remote Sensing Research

„Peer-Review“

„Best Practices“

Community-basierte Empfehlungen

Essentielle Bestandteile des Arbeitsprozesses

Teilnahme an wichtigen Community-Events

Nutzung des Prinzips Peer-Review

Internationalität

Analytics Experten

DataONE ***CODATA***

OGF ***NASA*** ***NIST***

Interesse aus South Africa

Einige Beispiele für Earth Science

Referenzierbare Papiere bei Peer-Review Community-Konferenzen & Tutorials …

… bspw. bei International Geoscience and Remote Sensing Symposium (IGARSS) 2014

Organisation und Teilnahme von “Big Data Sessions “ bei Community-Events…

… American Geophysical Union (AGU) 2013…

… European Geosciences Union (EGU) General Assembly 2014…

Talk: Research Data Alliance: Understanding Big Data Analytics Applications in Earth Science

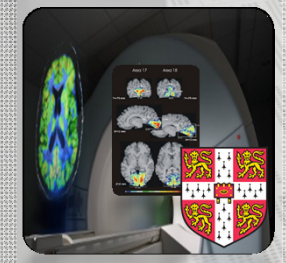
[10] EGU RDA 2014 Session

Big Data Analytics Interest Group

Weitere Wissenschaftliche Anwendungen

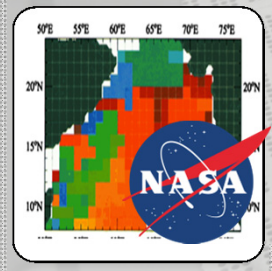
MARUM BREMEN

- Problem: „Outlier detection for automatic quality control“
- Große Anzahl Datensätze von Messungen (bspw. PANGAEA Kollektion)
- Tech: HPC/HTC (map-reduce?), Sybase In-DB Analytics?, SciDB?…



UoCAMBRIDGE

- Problem: „High Precision Radiotherapy Treatment“
- Kombinierte Analyse von Daten (CT Scans, X-Rays, MRI scans, PET images)
- Tech: HPC/HTC, In-Memory/NoSQL- Datebases – welche sinnvoll?, …



NASA - MSFC

- Problem: „Event tracking analytics“ (bspw. Entstehung von Somali Jets)
- Datensätze von Sateilliten (‘Suche Events mit wechselnden Geolocations‘)
- Tech: HPC/HTC (map-reduce?), Twister/Harp?, NASA software stacks,…

Big Data Analytics Interest Group

Weitere Punkte zum Arbeitsprozess

[11] RDA Big Data Analytics Web Page

Session-Qualität: Gelistete Vorträge mit PDF

Presentations - Day 1

Morris Riedel - Classification Techniques in Remote Sensing Research using Smart Data Analytics
- Forschungszentrum Jülich, Germany and University of Iceland, Reykjavik
- Remote sensing use case, classify satellite image pixels into land-cover classes (trees, soil, ...)
- Parallel support vector machine (SVM) technology comparison

Shabaz Memmon - Ultrascan and Brain Analytics
- Forschungszentrum Jülich, Germany
- Two use cases:
  - Ultracentrifugation experimentation in the analysis of biological and synthetic macromolecules
  - Human brain functionality understanding based on cross section block images
- Ultrascan (US3) based on MPI
- Random Forrests and SVM with RBF kernels

Analytics Experte

Geoffrey Fox - Data Analytics at Digital Science Center @SOIC
- Indiana University, Bloomington, USA
- Integration of HPC with the Apache Big Data Stack
- 16 different use cases

Presentations - Day 2

Wo Chang - RDA Big Data Activities
- National Institute for Standards and Technology (NIST), Gaithersburg, USA
- Presentation of the NIST Big Data Analytics Reference Architecture
- Fingerprint Analysis Use Case

NIST

Kuo Kwo-Sen - Automated Identification of Episodes of Earth Science Phenomena
- Bayesian & NASA, Maryland, USA
- In-array database analytics using SciDB
- Blizzard Observation Use Case

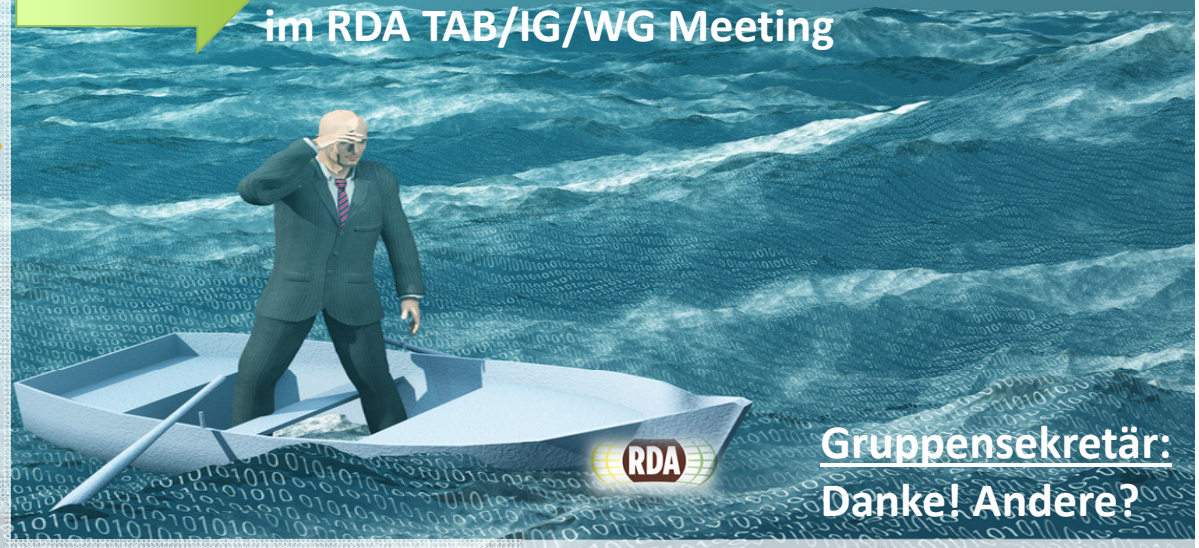
NASA

Peter Baumann - Use Case Array Databases
- Jacobs University, Munich, Germany
- Agile array analytics on top of the rasdaman array database
- Various use cases, including stock trading, social networks, climatology, HEP and genomes

Hugh Shanahan - NGS Transcriptomic Workflows
- Royal Holloway, University of London, UK
- NGS Transcriptomic Workflow from trace data to expemerimentation
- Sequencing pipeline and storage

Frank Seinstra - Big Compute meets Big Data
- Netherlands eScience Center, Amsterdam, The Netherlands
- eSTeP - eScience Technology Plattform (AEther, Xenon, ...), bridging science and industry
- Different use cases (supernova detection, climate research, ...)

Teilnahme & Vorschlag im letzten 4 Plenary im RDA TAB/IG/WG Meeting



Gruppensekretär: Danke! Andere?

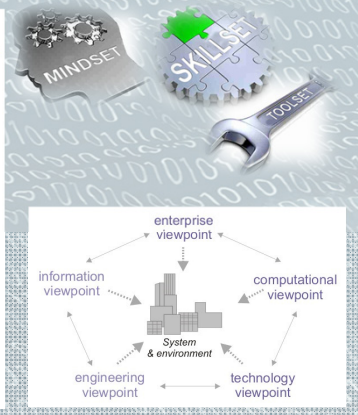
Each section below pertains to one RM-ODP viewpoint. First an explanatory introduction is given (in *italics*), then the Big Data Analytics use cases follow. (Please add your use cases by **using the template** and **along this schema** and **fit it into the appropriate section**!)

Enterprise viewpoint

The enterprise viewpoint focuses on the purpose, scope and policies for the system. It describes the scientific requirements and how to meet them, abstracting away from technical details.

Responsible section editor: Kuo Sen-Kwo **load-balance "admin work"**

Science domain use cases found relevant for Big Data Analytics:
- Event Analysis (Dr. Tom Clune, Dr. Kuo GSFC/NASA)
- Particle physics and radiotherapy (Michael Simmons and Charles Boulton, University of Cambridge)
- Research on Data Analytics for Automated Quality Control of Measurement Data (Morris Riedel, Shiraz Memon, Shahbaz Memon - Juelich Supercomputing Centre; Robert Huber - MARUM Bremen)
- Spatio-Temporal Data in the Earth Sciences (Peter Baumann, Jacobs University)
- Classification of land cover types of remote sensing satellite image datasets (Gabriele Cavallaro - University of Iceland, Morris Riedel - Juelich Supercomputing Centre)

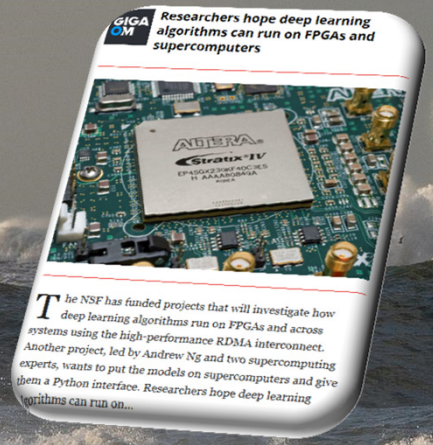


Aktualisierung Webseite (bspw. mit aktuellen Themen: ist für analytics das ISO Reference Model for Open Distributed Processing (RM-ODP) sinnvoll?

Big Data Analytics Interest Group

Nächste Schritte & Aktuelle Diskussionen

„Zuhören & Open Minded bleiben für neue Vorschläge“



- Voranbringen des Peer-review systems (Wer liest/prüft Analytics – Resultate, …)
- Weitere Communities einbringen (bspw. Earth Science Fokus, Medizin, andere …)
- Bessere Vernetzung mit anderen Gruppen (bspw. Terminologies and Foundations)
- Erweiterung der IG Richtung “Big Data“ (bspw. analytics nur noch als Teilbereich/WG)
- Diskussionen um die ISO RM-ODP Methode zur Beschreibung (mehr als CRISP-DM, …)
- Vorbereitung der Sessions im Plenary 5 in San Diego (mit anderen Gruppen, “Uptake“)

Sampling vs. Big Data

Parallelization!

Applied Statistics

Data Mining

Machine Learning Algorithms

Scientific Computing

new DBs

Training Data Scientists

Computational Scientist

Engineer

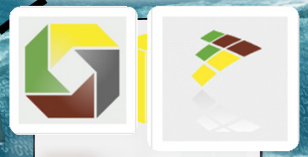
Data Miner

Software Engineer

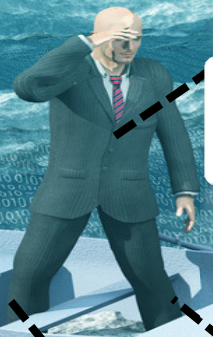
Statistician

Data Practitioner

Data Scientist



Many other RDA Groups



RDA

Insights

‘…and don‘t forget the big picture…‘

PhD Student works with NASA on SciDB Analytics

JÜLICH FORSCHUNGSZENTRUM

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

Statistical Data Mining Course

HPC – B(ig Data) Course

HPC – A(advanced) Scientific Computing Course

Data Scientists with skills of various fields

Danke für Ihre Aufmerksamkeit & Dank an RDA für „Platform“

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